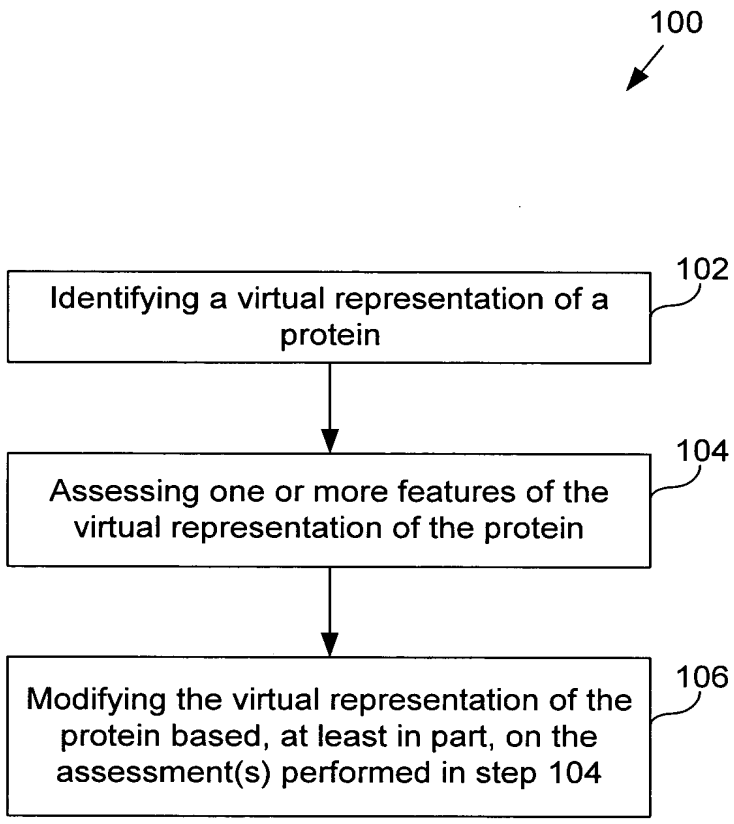

FIG. 1

0203-73.vsd/1

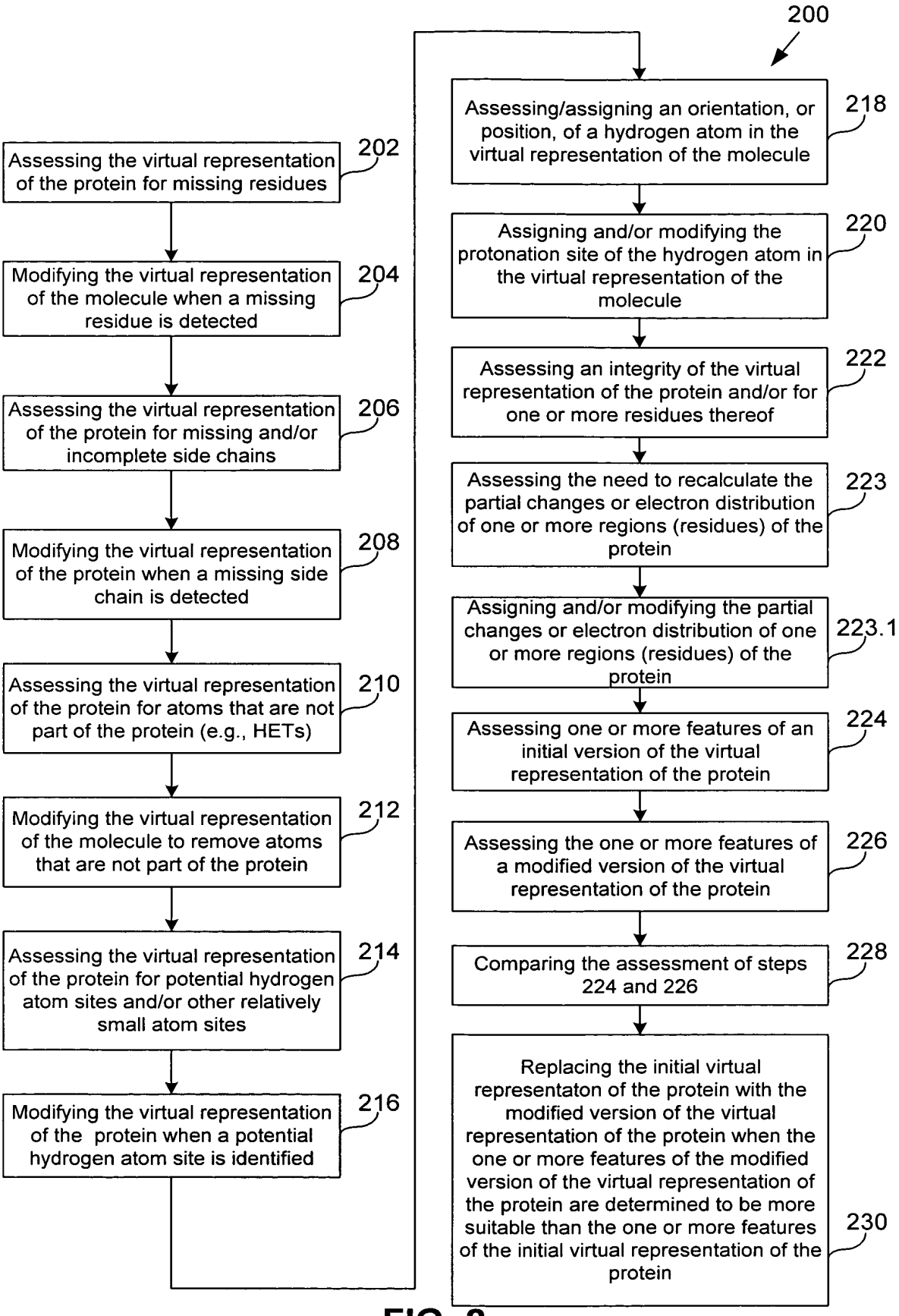

FIG. 2

0203-73.vsd/2

FIG. 3A

PDB
PROTEIN DATA BANK

Structure Explorer - 1AIK

[redacted]

Title **Hiv Gp41 Core Structure**
Classification **Glycoprotein**
Compound **Mol_Id: 1; Molecule: Hiv-1 Gp41 Glycoprotein; Chain: N, C; Fragment: Protease-Resistant Core; Biological_Unit: Trimer; Other_Details: N36 and C34 Are Synthetic Peptides**
Exp. Method **X-ray Diffraction**

Download/Display File

Summary Information
View Structure
Download/Display File
Structural Neighbors
Geometry
Other Sources
Sequence Details

[redacted]
SearchLite SearchFields

Save full entry to disk

```
HEADER    GLYCOPROTEIN                                20-APR-97   1AIK
TITLE     HIV GP41 CORE STRUCTURE
COMPND    MOL_ID: 1;
COMPND   2 MOLECULE: HIV-1 GP41 GLYCOPROTEIN;
COMPND   3 CHAIN: N, C;
COMPND   4 FRAGMENT: PROTEASE-RESISTANT CORE;
COMPND   5 BIOLOGICAL_UNIT: TRIMER;
COMPND   6 OTHER_DETAILS: N36 AND C34 ARE SYNTHETIC PEPTIDES
SOURCE    MOL_ID: 1;
SOURCE   2 ORGANISM_SCIENTIFIC: HUMAN IMMUNODEFICIENCY VIRUS TYPE 1;
SOURCE   3 STRAIN: HXB2;
SOURCE   4 CELLULAR_LOCATION: VIRAL MEMBRANE
KEYWDS    HIV, GP41, ENVELOPE GLYCOPROTEIN, RETROVIRUS
EXPDTA    X-RAY DIFFRACTION
AUTHOR    D.C.CHAN,D.FASS,J.M.BERGER,P.S.KIM
REVDAT   1   16-JUN-97 1AIK    0
REMARK    1
REMARK   1 REFERENCE 1
REMARK   1  AUTH    D.C.CHAN,D.FASS,J.M.BERGER,P.S.KIM
REMARK   1  TITL    CORE STRUCTURE OF GP41 FROM THE HIV ENVELOPE
REMARK   1  TITL 2 GLYCOPROTEIN
REMARK   1  REF     CELL(CAMBRIDGE,MASS.)          V.  89    263 1997
REMARK   1  REFN    ASTM CELLB5  US ISSN 0092-8674                  0998
REMARK    2
REMARK   2 RESOLUTION. 2.0  ANGSTROMS.
REMARK    3
REMARK   3 REFINEMENT.
REMARK   3   PROGRAM     : X-PLOR 3.851
```

```
REMARK   3   AUTHORS     : BRUNGER
REMARK   3
REMARK   3  DATA USED IN REFINEMENT.
REMARK   3   RESOLUTION RANGE HIGH (ANGSTROMS) : 2.0
REMARK   3   RESOLUTION RANGE LOW  (ANGSTROMS) : 12.0
REMARK   3   DATA CUTOFF            (SIGMA(F)) : 2.0
REMARK   3   DATA CUTOFF HIGH         (ABS(F)) : 100000000.
REMARK   3   DATA CUTOFF LOW          (ABS(F)) : NULL
REMARK   3   COMPLETENESS (WORKING+TEST)   (%) : 96.5
REMARK   3   NUMBER OF REFLECTIONS             : 5683
REMARK   3
REMARK   3  FIT TO DATA USED IN REFINEMENT.
REMARK   3   CROSS-VALIDATION METHOD           : THROUGHOUT
REMARK   3   FREE R VALUE TEST SET SELECTION   : RANDOM
REMARK   3   R VALUE            (WORKING SET) : 0.238
REMARK   3   FREE R VALUE                      : 0.266
REMARK   3   FREE R VALUE TEST SET SIZE   (%) : 7.12
REMARK   3   FREE R VALUE TEST SET COUNT       : 371
REMARK   3   ESTIMATED ERROR OF FREE R VALUE   : NULL
REMARK   3
REMARK   3  FIT IN THE HIGHEST RESOLUTION BIN.
REMARK   3   TOTAL NUMBER OF BINS USED           : NULL
REMARK   3   BIN RESOLUTION RANGE HIGH       (A) : NULL
REMARK   3   BIN RESOLUTION RANGE LOW        (A) : NULL
REMARK   3   BIN COMPLETENESS (WORKING+TEST) (%) : NULL
REMARK   3   REFLECTIONS IN BIN    (WORKING SET) : NULL
REMARK   3   BIN R VALUE           (WORKING SET) : NULL
REMARK   3   BIN FREE R VALUE                    : NULL
REMARK   3   BIN FREE R VALUE TEST SET SIZE  (%) : NULL
REMARK   3   BIN FREE R VALUE TEST SET COUNT     : NULL
REMARK   3   ESTIMATED ERROR OF BIN FREE R VALUE : NULL
REMARK   3
REMARK   3  NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK   3   PROTEIN ATOMS            : 596
REMARK   3   NUCLEIC ACID ATOMS       : 0
REMARK   3   HETEROGEN ATOMS          : 0
REMARK   3   SOLVENT ATOMS            : 43
REMARK   3
REMARK   3  B VALUES.
REMARK   3   FROM WILSON PLOT           (A**2) : NULL
REMARK   3   MEAN B VALUE      (OVERALL, A**2) : NULL
REMARK   3   OVERALL ANISOTROPIC B VALUE.
REMARK   3    B11 (A**2) : NULL
```

```
REMARK   3    B22 (A**2) : NULL
REMARK   3    B33 (A**2) : NULL
REMARK   3    B12 (A**2) : NULL
REMARK   3    B13 (A**2) : NULL
REMARK   3    B23 (A**2) : NULL
REMARK   3
REMARK   3  ESTIMATED COORDINATE ERROR.
REMARK   3   ESD FROM LUZZATI PLOT          (A) : NULL
REMARK   3   ESD FROM SIGMAA                (A) : NULL
REMARK   3   LOW RESOLUTION CUTOFF          (A) : NULL
REMARK   3
REMARK   3  CROSS-VALIDATED ESTIMATED COORDINATE ERROR.
REMARK   3   ESD FROM C-V LUZZATI PLOT      (A) : NULL
REMARK   3   ESD FROM C-V SIGMAA            (A) : NULL
REMARK   3
REMARK   3  RMS DEVIATIONS FROM IDEAL VALUES.
REMARK   3   BOND LENGTHS                   (A) : 0.014
REMARK   3   BOND ANGLES             (DEGREES) : 2.742
REMARK   3   DIHEDRAL ANGLES         (DEGREES) : NULL
REMARK   3   IMPROPER ANGLES         (DEGREES) : NULL
REMARK   3
REMARK   3  ISOTROPIC THERMAL MODEL : NULL
REMARK   3
REMARK   3  ISOTROPIC THERMAL FACTOR RESTRAINTS.     RMS     SIGMA
REMARK   3   MAIN-CHAIN BOND              (A**2) : NULL  ; NULL
REMARK   3   MAIN-CHAIN ANGLE             (A**2) : NULL  ; NULL
REMARK   3   SIDE-CHAIN BOND              (A**2) : NULL  ; NULL
REMARK   3   SIDE-CHAIN ANGLE             (A**2) : NULL  ; NULL
REMARK   3
REMARK   3  NCS MODEL : NULL
REMARK   3
REMARK   3  NCS RESTRAINTS.                          RMS   SIGMA/WEIGHT
REMARK   3   GROUP  1  POSITIONAL              (A) : NULL  ; NULL
REMARK   3   GROUP  1  B-FACTOR            (A**2) : NULL  ; NULL
REMARK   3
REMARK   3  PARAMETER FILE  1  : NULL
REMARK   3  PARAMETER FILE  2  : NULL
REMARK   3  TOPOLOGY FILE  1   : NULL
REMARK   3  TOPOLOGY FILE  2   : NULL
REMARK   3
REMARK   3  OTHER REFINEMENT REMARKS: NULL
REMARK   4
REMARK   4 1AIK COMPLIES WITH FORMAT V. 2.2, 16-DEC-1996
```

```
REMARK   6
REMARK   6 C-TERMINAL NH2 NOT IN ATOM LIST FOR BOTH CHAINS.
REMARK 200
REMARK 200 EXPERIMENTAL DETAILS
REMARK 200  EXPERIMENT TYPE                : X-RAY DIFFRACTION
REMARK 200  DATE OF DATA COLLECTION        : MAR-1997
REMARK 200  TEMPERATURE           (KELVIN) : 100
REMARK 200  PH                             : 6.0
REMARK 200  NUMBER OF CRYSTALS USED        : 1
REMARK 200
REMARK 200  SYNCHROTRON              (Y/N) : N
REMARK 200  RADIATION SOURCE               : NULL
REMARK 200  BEAMLINE                       : NULL
REMARK 200  X-RAY GENERATOR MODEL          : RIGAKU RU200
REMARK 200  MONOCHROMATIC OR LAUE    (M/L) : M
REMARK 200  WAVELENGTH OR RANGE        (A) : 1.5418
REMARK 200  MONOCHROMATOR                  : NULL
REMARK 200  OPTICS                         : MIRRORS
REMARK 200
REMARK 200  DETECTOR TYPE                  : R-AXIS IIC
REMARK 200  DETECTOR MANUFACTURER          : RIGAKU
REMARK 200  INTENSITY-INTEGRATION SOFTWARE : DENZO
REMARK 200  DATA SCALING SOFTWARE          : SCALEPACK
REMARK 200
REMARK 200  NUMBER OF UNIQUE REFLECTIONS   : 5287
REMARK 200  RESOLUTION RANGE HIGH      (A) : 2.0
REMARK 200  RESOLUTION RANGE LOW       (A) : 20.0
REMARK 200  REJECTION CRITERIA  (SIGMA(I)) : 1.5
REMARK 200
REMARK 200 OVERALL.
REMARK 200  COMPLETENESS FOR RANGE     (%) : 96.5
REMARK 200  DATA REDUNDANCY                : NULL
REMARK 200  R MERGE                    (I) : NULL
REMARK 200  R SYM                      (I) : 0.054
REMARK 200  <I/SIGMA(I)> FOR THE DATA SET  : 18.4
REMARK 200
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.
REMARK 200  HIGHEST RESOLUTION SHELL, RANGE HIGH (A) : 2.00
REMARK 200  HIGHEST RESOLUTION SHELL, RANGE LOW  (A) : 2.07
REMARK 200  COMPLETENESS FOR SHELL     (%) : 98.9
REMARK 200  DATA REDUNDANCY IN SHELL       : NULL
REMARK 200  R MERGE FOR SHELL          (I) : NULL
REMARK 200  R SYM FOR SHELL            (I) : 0.263
```

```
REMARK 200  <I/SIGMA(I)> FOR SHELL         : 5.4
REMARK 200
REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: MAD
REMARK 200 SOFTWARE USED: CCP4 SUITE
REMARK 200 STARTING MODEL: NULL
REMARK 200
REMARK 200 REMARK: DATA AT NSLS USED MAD METHODS.  DATA COLLECTED ON
REMARK 200 AN OSMIUM-SOAK CRYSTAL AT WAVELENGTHS 1.1398, 1.1396,
REMARK 200 1.1344, AND 1.1406 ANGSTROMS.
REMARK 280
REMARK 280 CRYSTAL
REMARK 280 SOLVENT CONTENT, VS   (%): 46.
REMARK 280 MATTHEWS COEFFICIENT, VM (ANGSTROMS**3/DA): NULL
REMARK 280
REMARK 280 CRYSTALLIZATION CONDITIONS: A 10 MG/ML STOCK WAS DILUTED
REMARK 280 1:1 IN A SITTING DROP WITH 80 MM NH4CL, 20% PEG200, AND
REMARK 280 50% ISOPROPANOL, AND THEN ALLOWED TO EQUILIBRATE AGAINST
REMARK 280 80 MM NH4CL, 20% PEG200, AND 30% ISOPROPANOL.
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY
REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP: P 3 2 1
REMARK 290
REMARK 290      SYMOP   SYMMETRY
REMARK 290     NNNMMM   OPERATOR
REMARK 290       1555   X,Y,Z
REMARK 290       2555   -Y,X-Y,Z
REMARK 290       3555   Y-X,-X,Z
REMARK 290       4555   Y,X,-Z
REMARK 290       5555   X-Y,-Y,-Z
REMARK 290       6555   -X,Y-X,-Z
REMARK 290
REMARK 290     WHERE NNN -> OPERATOR NUMBER
REMARK 290           MMM -> TRANSLATION VECTOR
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS
REMARK 290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM
REMARK 290 RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY
REMARK 290 RELATED MOLECULES.
REMARK 290   SMTRY1   1  1.000000  0.000000  0.000000        0.00000
REMARK 290   SMTRY2   1  0.000000  1.000000  0.000000        0.00000
REMARK 290   SMTRY3   1  0.000000  0.000000  1.000000        0.00000
REMARK 290   SMTRY1   2 -0.500021 -0.866016  0.000000        0.00000
REMARK 290   SMTRY2   2  0.866035 -0.499979  0.000000        0.00000
```

FIG. 3F


```
REMARK 290   SMTRY3   2  0.000000  0.000000  1.000000        0.00000
REMARK 290   SMTRY1   3 -0.499979  0.866016  0.000000        0.00000
REMARK 290   SMTRY2   3 -0.866035 -0.500021  0.000000        0.00000
REMARK 290   SMTRY3   3  0.000000  0.000000  1.000000        0.00000
REMARK 290   SMTRY1   4 -0.500021  0.865991  0.000000        0.00000
REMARK 290   SMTRY2   4  0.866035  0.500021  0.000000        0.00000
REMARK 290   SMTRY3   4  0.000000  0.000000 -1.000000        0.00000
REMARK 290   SMTRY1   5  1.000000  0.000050  0.000000        0.00000
REMARK 290   SMTRY2   5  0.000000 -1.000000  0.000000        0.00000
REMARK 290   SMTRY3   5  0.000000  0.000000 -1.000000        0.00000
REMARK 290   SMTRY1   6 -0.499979 -0.866041  0.000000        0.00000
REMARK 290   SMTRY2   6 -0.866035  0.499979  0.000000        0.00000
REMARK 290   SMTRY3   6  0.000000  0.000000 -1.000000        0.00000
REMARK 290
REMARK 290 REMARK: NULL
REMARK 999
REMARK 999 SEQUENCE
REMARK 999 1AIK  C    SWS     P04582       1 -   621 NOT IN ATOMS LIST
REMARK 999 1AIK  C    SWS     P04582     657 -   851 NOT IN ATOMS LIST
REMARK 999 1AIK  N    SWS     P19551       1 -   542 NOT IN ATOMS LIST
REMARK 999 1AIK  N    SWS     P19551     580 -   853 NOT IN ATOMS LIST
DBREF  1AIK C    0   661  SWS    P04582   ENV_HV1B8      622    656
DBREF  1AIK N    0   581  SWS    P19551   ENV_HV1MF      543    579
SEQADV 1AIK ACE C    0  SWS  P04582    THR   622 CONFLICT
SEQADV 1AIK ACE N    0  SWS  P19551    LEU   543 CONFLICT
SEQRES   1 N   38  ACE SER GLY ILE VAL GLN GLN GLN ASN ASN LEU LEU ARG
SEQRES   2 N   38  ALA ILE GLU ALA GLN GLN HIS LEU LEU GLN LEU THR VAL
SEQRES   3 N   38  TRP GLY ILE LYS GLN LEU GLN ALA ARG ILE LEU NH2
SEQRES   1 C   36  ACE TRP MET GLU TRP ASP ARG GLU ILE ASN ASN TYR THR
SEQRES   2 C   36  SER LEU ILE HIS SER LEU ILE GLU GLU SER GLN ASN GLN
SEQRES   3 C   36  GLN GLU LYS ASN GLU GLN GLU LEU LEU NH2
HET    ACE  N   0       3
HET    ACE  C   0       3
HETNAM     ACE ACETYL GROUP
FORMUL   1  ACE    C2 H3 O1
FORMUL   2  ACE    C2 H3 O1
FORMUL   3  HOH   *43(H2 O1)
HELIX    1   1 GLY N  547  ALA N  578  1                                  32
HELIX    2   2 MET C  629  GLU C  659  1                                  31
LINK         C   ACE N   0                 N   SER N 546
LINK         C   ACE C   0                 N   TRP C 628
CRYST1   49.500   49.500   55.300  90.00  90.00 120.00 P 3 2 1       6
ORIGX1      1.000000  0.000000  0.000000        0.00000
```

FIG. 3G

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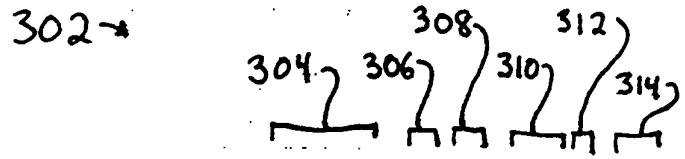
```
ORIGX2      0.000000  1.000000  0.000000        0.00000
ORIGX3      0.000000  0.000000  1.000000        0.00000
SCALE1      0.020202  0.011664  0.000000        0.00000
SCALE2      0.000000  0.023327  0.000000        0.00000
SCALE3      0.000000  0.000000  0.018083        0.00000
HETATM    1  C   ACE N   0      19.211  14.270 -17.472  1.00 56.26           C
HETATM    2  O   ACE N   0      19.488  14.580 -16.305  1.00 56.37           O
HETATM    3  CH3 ACE N   0      20.273  14.045 -18.531  1.00 56.01           C
ATOM      4  N   SER N 546      17.955  14.014 -17.827  1.00 56.49           N
ATOM      5  CA  SER N 546      16.876  14.392 -16.942  1.00 56.15           C
ATOM      6  C   SER N 546      16.909  13.631 -15.655  1.00 56.24           C
ATOM      7  O   SER N 546      16.736  14.255 -14.615  1.00 57.67           O
ATOM      8  CB  SER N 546      15.525  14.172 -17.546  1.00 56.05           C
ATOM      9  OG  SER N 546      15.498  12.815 -17.842  1.00 57.84           O
ATOM     10  H   SER N 546      17.816  13.501 -18.652  1.00  0.00           H
ATOM     11  HG  SER N 546      15.988  12.455 -18.582  1.00  0.00           H
ATOM     12  N   GLY N 547      17.181  12.316 -15.724  1.00 55.59           N
ATOM     13  CA  GLY N 547      17.202  11.414 -14.570  1.00 53.04           C
ATOM     14  C   GLY N 547      18.299  11.783 -13.596  1.00 51.70           C
ATOM     15  O   GLY N 547      18.147  11.667 -12.391  1.00 50.76           O
ATOM     16  H   GLY N 547      17.409  11.945 -16.618  1.00  0.00           H
ATOM     17  N   ILE N 548      19.399  12.280 -14.145  1.00 51.57           N
ATOM     18  CA  ILE N 548      20.551  12.815 -13.425  1.00 52.14           C
ATOM     19  C   ILE N 548      20.218  14.116 -12.696  1.00 51.31           C
ATOM     20  O   ILE N 548      20.543  14.273 -11.519  1.00 50.83           O
ATOM     21  CB  ILE N 548      21.693  13.043 -14.436  1.00 54.22           C
ATOM     22  CG1 ILE N 548      22.120  11.712 -15.087  1.00 54.58           C
ATOM     23  CG2 ILE N 548      22.861  13.705 -13.721  1.00 55.25           C
ATOM     24  CD1 ILE N 548      23.126  11.909 -16.234  1.00 56.29           C
ATOM     25  H   ILE N 548      19.445  12.272 -15.118  1.00  0.00           H
ATOM     26  N   VAL N 549      19.590  15.054 -13.393  1.00 50.93           N
ATOM     27  CA  VAL N 549      19.093  16.291 -12.786  1.00 50.79           C
ATOM     28  C   VAL N 549      18.036  15.977 -11.726  1.00 50.36           C
ATOM     29  O   VAL N 549      17.992  16.598 -10.674  1.00 51.60           O
ATOM     30  CB  VAL N 549      18.451  17.196 -13.841  1.00 52.28           C
ATOM     31  CG1 VAL N 549      17.814  18.437 -13.226  1.00 54.97           C
ATOM     32  CG2 VAL N 549      19.539  17.650 -14.780  1.00 51.05           C
ATOM     33  H   VAL N 549      19.486  14.911 -14.360  1.00  0.00           H
ATOM     34  N   GLN N 550      17.187  15.030 -12.001  1.00 49.13           N
ATOM     35  CA  GLN N 550      16.176  14.508 -11.109  1.00 49.23           C
ATOM     36  C   GLN N 550      16.843  13.895  -9.861  1.00 48.50           C
ATOM     37  O   GLN N 550      16.520  14.236  -8.736  1.00 47.94           O
ATOM     38  CB  GLN N 550      15.452  13.398 -11.814  1.00 52.96           C
```

FIG. 3H



HETATM	1	C	ACE	N	0	19.211	14.270	-17.472	1.00	56.26	C
HETATM	2	O	ACE	N	0	19.488	14.580	-16.305	1.00	56.37	O
HETATM	3	CH3	ACE	N	0	20.273	14.045	-18.531	1.00	56.01	C
ATOM	4	N	SER	N	546	17.955	14.014	-17.827	1.00	56.49	N
ATOM	5	CA	SER	N	546	16.876	14.392	-16.942	1.00	56.15	C
ATOM	6	C	SER	N	546	16.909	13.631	-15.655	1.00	56.24	C
ATOM	7	O	SER	N	546	16.736	14.255	-14.615	1.00	57.67	O
ATOM	8	CB	SER	N	546	15.525	14.172	-17.546	1.00	56.05	C
ATOM	9	OG	SER	N	546	15.498	12.815	-17.842	1.00	57.84	O
ATOM	10	H	SER	N	546	17.816	13.501	-18.652	1.00	0.00	H
ATOM	11	HG	SER	N	546	15.988	12.455	-18.582	1.00	0.00	H
ATOM	12	N	GLY	N	547	17.181	12.316	-15.724	1.00	55.59	N
ATOM	13	CA	GLY	N	547	17.202	11.414	-14.570	1.00	53.04	C
ATOM	14	C	GLY	N	547	18.299	11.783	-13.596	1.00	51.70	C
ATOM	15	O	GLY	N	547	18.147	11.667	-12.391	1.00	50.76	O
ATOM	16	H	GLY	N	547	17.409	11.945	-16.618	1.00	0.00	H
ATOM	17	N	ILE	N	548	19.399	12.280	-14.145	1.00	51.57	N
ATOM	18	CA	ILE	N	548	20.551	12.815	-13.425	1.00	52.14	C
ATOM	19	C	ILE	N	548	20.218	14.116	-12.696	1.00	51.31	C
ATOM	20	O	ILE	N	548	20.543	14.273	-11.519	1.00	50.83	O
ATOM	21	CB	ILE	N	548	21.693	13.043	-14.436	1.00	54.22	C
ATOM	22	CG1	ILE	N	548	22.120	11.712	-15.087	1.00	54.58	C
ATOM	23	CG2	ILE	N	548	22.861	13.705	-13.721	1.00	55.25	C
ATOM	24	CD1	ILE	N	548	23.126	11.909	-16.234	1.00	56.29	C
ATOM	25	H	ILE	N	548	19.445	12.272	-15.118	1.00	0.00	H
ATOM	26	N	VAL	N	549	19.590	15.054	-13.393	1.00	50.93	N
ATOM	27	CA	VAL	N	549	19.093	16.291	-12.786	1.00	50.79	C
ATOM	28	C	VAL	N	549	18.036	15.977	-11.726	1.00	50.36	C
ATOM	29	O	VAL	N	549	17.992	16.598	-10.674	1.00	51.60	O
ATOM	30	CB	VAL	N	549	18.451	17.196	-13.841	1.00	52.28	C
ATOM	31	CG1	VAL	N	549	17.814	18.437	-13.226	1.00	54.97	C
ATOM	32	CG2	VAL	N	549	19.539	17.650	-14.780	1.00	51.05	C
ATOM	33	H	VAL	N	549	19.486	14.911	-14.360	1.00	0.00	H
ATOM	34	N	GLN	N	550	17.187	15.030	-12.001	1.00	49.13	N
ATOM	35	CA	GLN	N	550	16.176	14.508	-11.109	1.00	49.23	C
ATOM	36	C	GLN	N	550	16.843	13.895	-9.861	1.00	48.50	C
ATOM	37	O	GLN	N	550	16.520	14.236	-8.736	1.00	47.94	O
ATOM	38	CB	GLN	N	550	15.452	13.398	-11.814	1.00	52.96	C

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```
TITLE     gp41n3.mod
REMARK 987       26.67       25.42       53.56
ATOM      1   C   ACE A   0      -5.539   -0.020  -17.472
ATOM      2   O   ACE A   0      -5.262    0.290  -16.305
ATOM      3   CH3 ACE A   0      -4.477   -0.245  -18.531
ATOM      4 1HH3 ACE A   0      -3.490   -0.091  -18.094
ATOM      5 2HH3 ACE A   0      -4.626    0.459  -19.350
ATOM      6 3HH3 ACE A   0      -4.552   -1.264  -18.910
ATOM      7   N   SER A 546      -6.795   -0.276  -17.827
ATOM      8   CA  SER A 546      -7.874    0.102  -16.942
ATOM      9   C   SER A 546      -7.841   -0.659  -15.655
ATOM     10   O   SER A 546      -8.014   -0.035  -14.615
ATOM     11   CB  SER A 546      -9.225   -0.118  -17.546
ATOM     12   OG  SER A 546      -9.252   -1.475  -17.842
ATOM     13   H   SER A 546      -6.993   -0.730  -18.707
ATOM     14   HA  SER A 546      -7.718    1.166  -16.762
ATOM     15   HB2 SER A 546      -9.345    0.477  -18.451
ATOM     16   HB3 SER A 546     -10.012    0.138  -16.836
ATOM     17   HG  SER A 546     -10.097   -1.699  -18.238
ATOM     18   N   GLY A 547      -7.569   -1.974  -15.724
ATOM     19   CA  GLY A 547      -7.548   -2.876  -14.570
ATOM     20   C   GLY A 547      -6.451   -2.507  -13.596
ATOM     21   O   GLY A 547      -6.603   -2.623  -12.391
ATOM     22   H   GLY A 547      -7.365   -2.366  -16.632
ATOM     23   HA2 GLY A 547      -7.382   -3.895  -14.920
ATOM     24   HA3 GLY A 547      -8.509   -2.819  -14.059
ATOM     25   N   ILE A 548      -5.351   -2.010  -14.145
ATOM     26   CA  ILE A 548      -4.199   -1.475  -13.425
ATOM     27   C   ILE A 548      -4.532   -0.174  -12.696
ATOM     28   O   ILE A 548      -4.207   -0.017  -11.519
ATOM     29   CB  ILE A 548      -3.057   -1.247  -14.436
ATOM     30   CG1 ILE A 548      -2.630   -2.578  -15.087
ATOM     31   CG2 ILE A 548      -1.889   -0.585  -13.721
ATOM     32   CD1 ILE A 548      -1.624   -2.381  -16.234
ATOM     33   H   ILE A 548      -5.306   -2.001  -15.154
ATOM     34   HA  ILE A 548      -3.897   -2.193  -12.663
ATOM     35   HB  ILE A 548      -3.403   -0.592  -15.236
ATOM     36 2HG1 ILE A 548      -3.517   -3.073  -15.482
ATOM     37 3HG1 ILE A 548      -2.171   -3.208  -14.325
ATOM     38 1HG2 ILE A 548      -1.076   -0.420  -14.429
ATOM     39 2HG2 ILE A 548      -1.543   -1.232  -12.915
ATOM     40 3HG2 ILE A 548      -2.211    0.371  -13.307
ATOM     41 1HD1 ILE A 548      -1.359   -3.351  -16.655
ATOM     42 2HD1 ILE A 548      -0.727   -1.893  -15.851
ATOM     43 3HD1 ILE A 548      -2.073   -1.759  -17.008
ATOM     44   N   VAL A 549      -5.160    0.764  -13.393
ATOM     45   CA  VAL A 549      -5.657    2.001  -12.786
ATOM     46   C   VAL A 549      -6.714    1.687  -11.726
ATOM     47   O   VAL A 549      -6.758    2.308  -10.674
ATOM     48   CB  VAL A 549      -6.299    2.906  -13.841
ATOM     49   CG1 VAL A 549      -6.936    4.147  -13.226
ATOM     50   CG2 VAL A 549      -5.211    3.360  -14.780
ATOM     51   H   VAL A 549      -5.301    0.619  -14.382
ATOM     52   HA  VAL A 549      -4.805    2.508  -12.333
ATOM     53   HB  VAL A 549      -7.080    2.340  -14.348
ATOM     54 1HG1 VAL A 549      -7.378    4.757  -14.014
ATOM     55 2HG1 VAL A 549      -6.174    4.725  -12.703
```

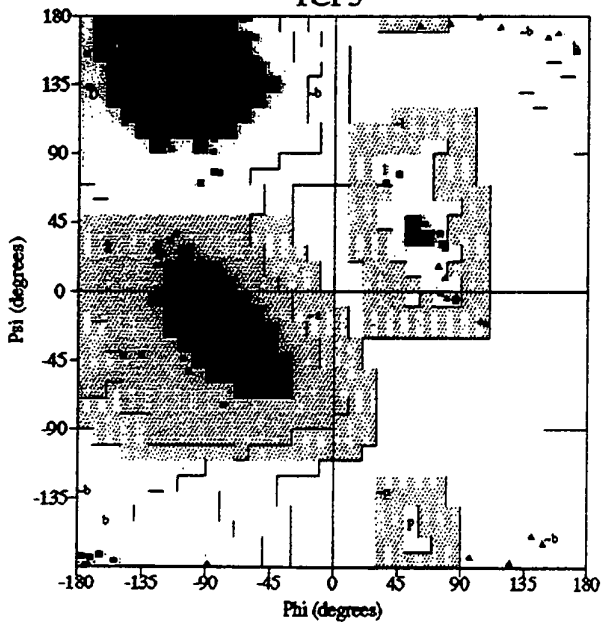
404

FIG. 4

PROCHECK

Ramachandran Plot

1CP3



Plot statistics

Residues in most favoured regions [A,B,L]	383	90.8%
Residues in additional allowed regions [a,b,l,p]	39	9.2%
Residues in generously allowed regions [~a,~b,~l,~p]	0	0.0%
Residues in disallowed regions	0	0.0%
Number of non-glycine and non-proline residues	422	100.0%
Number of end-residues (excl. Gly and Pro)	12	
Number of glycine residues (shown as triangles)	26	
Number of proline residues	12	
Total number of residues	472	

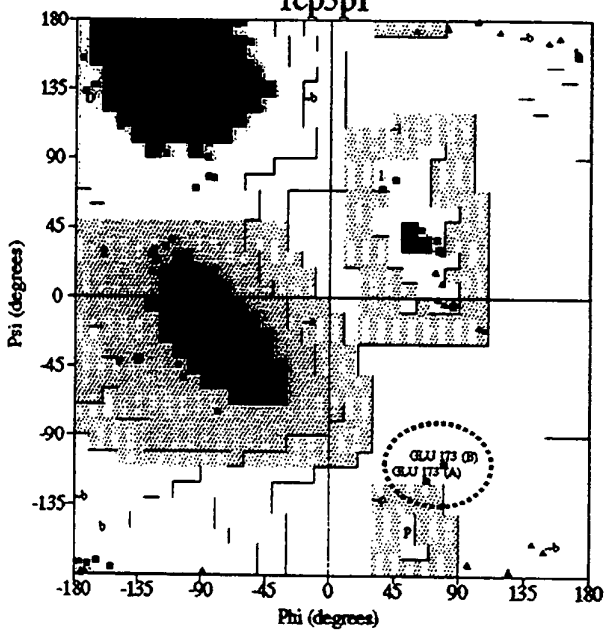
Based on an analysis of 118 structures of resolution of at least 2.0 Angstroms and R-factor no greater than 20%, a good quality model would be expected to have over 90% in the most favoured regions.

FIG. 5A

PROCHECK

Ramachandran Plot

1cp3p1



Plot statistics

Residues in most favoured regions [A,B,L]	378	89.6%
Residues in additional allowed regions [a,b,l,p]	42	10.0%
Residues in generously allowed regions [~a,~b,~l,~p]	0	0.0%
Residues in disallowed regions	2	0.5%
Number of non-glycine and non-proline residues	422	100.0%
Number of end-residues (excl. Gly and Pro)	8	
Number of glycine residues (shown as triangles)	26	
Number of proline residues	12	
Total number of residues	468	

Based on an analysis of 118 structures of resolution of at least 2.0 Angstroms and R-factor no greater than 20%, a good quality model would be expected to have over 90% in the most favoured regions.

FIG. 5B

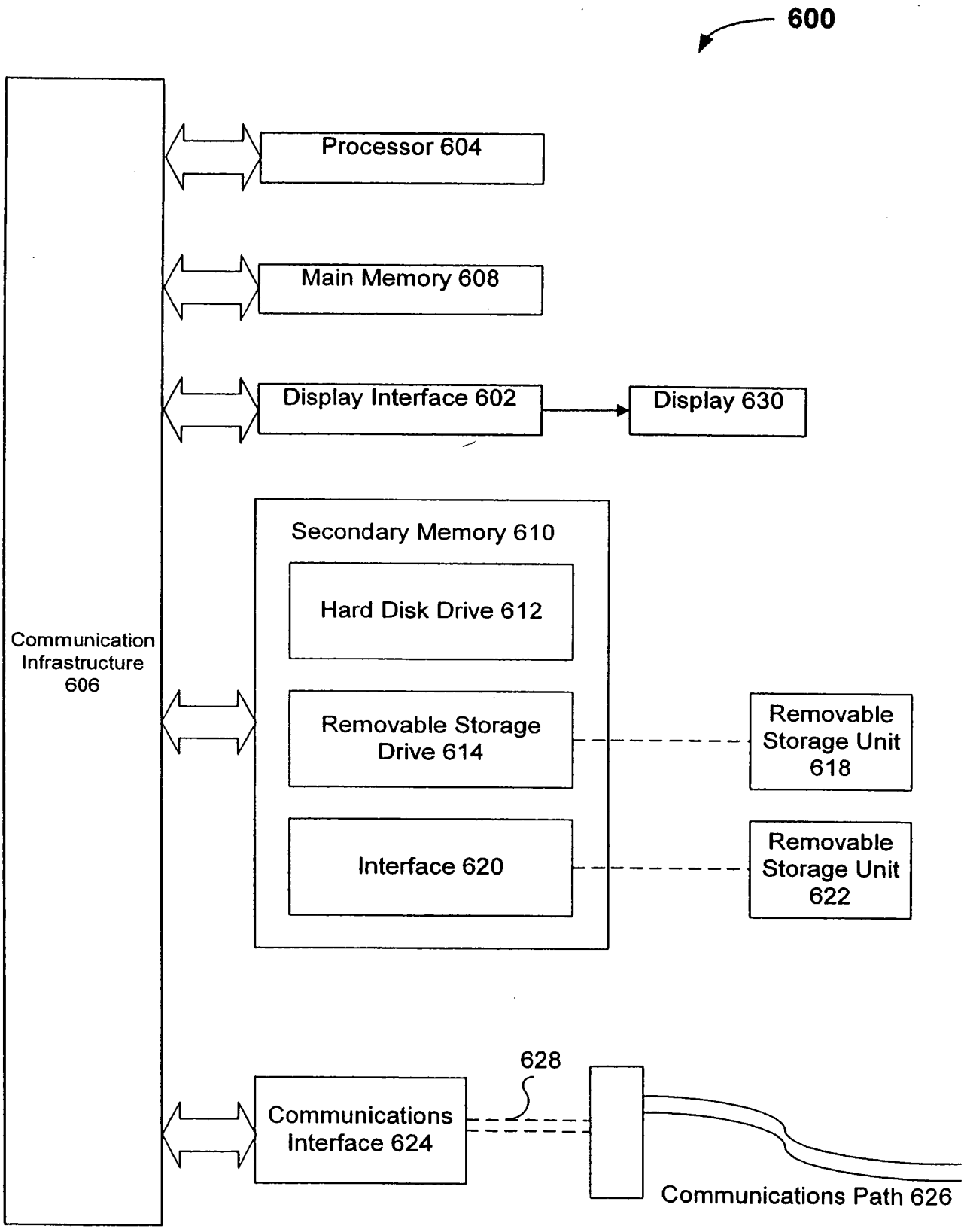


FIG. 6

computer.vsd/1

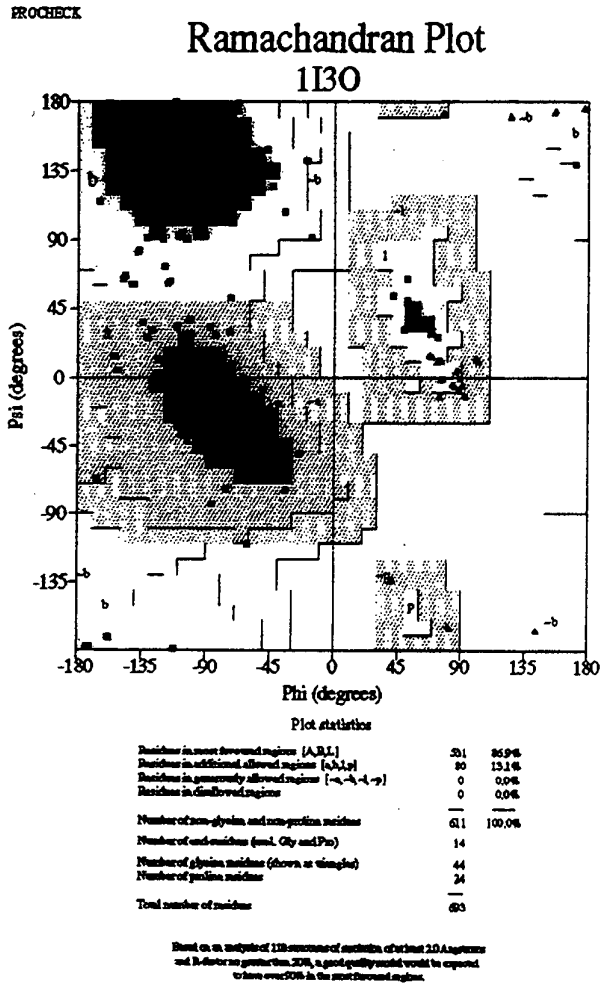

PROCHECK
Ramachandran Plot
1I3O
Psi (degrees)
Phi (degrees)
180
135
90
45
0
-45
-90
-135
-180
Plot statistics

FIG. 7A

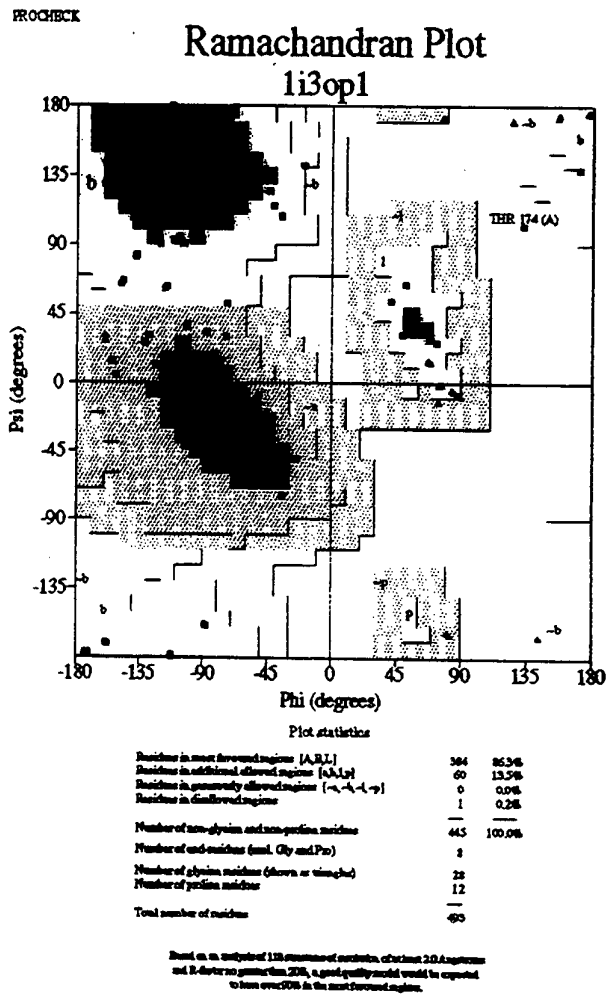

PROCHECK
Ramachandran Plot
1i3op1
THR
Psi (degrees)
Phi (degrees)
180
135
90
45
0
-45
-90
-135
-180
Plot statistics

FIG. 7B

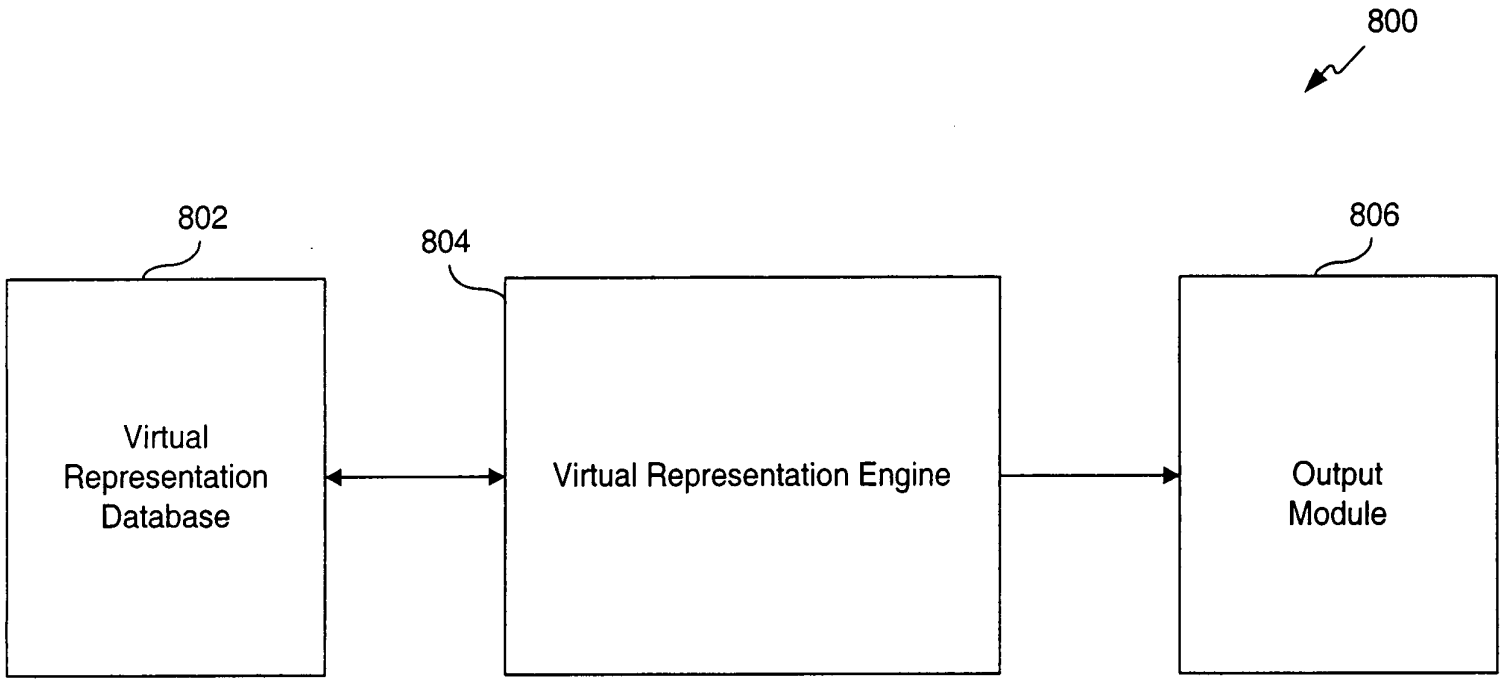
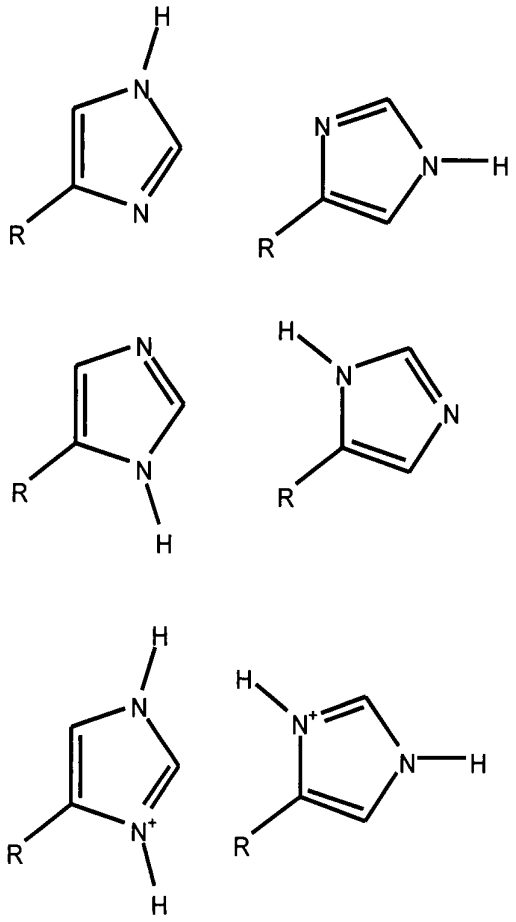
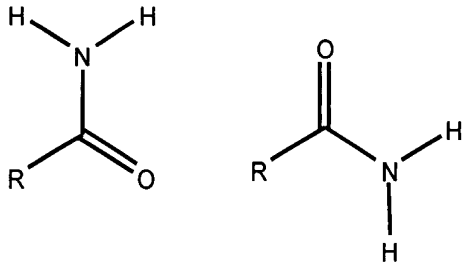

800
802
804
806
Virtual Representation Database
Virtual Representation Engine
Output Module

FIG. 8

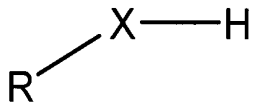
Histidine Termini
(4 neutral conformers, 2 protonated conformers, as appropriate)



Asparagine & Glutamine Residue Termini
(two conformations as shown below)



Tyrosine, Serine, Cysteine, Threonine Termini
(multiple rotor states around the R-X bond)



X = O, S

The R in each case is the remainder of specific residue under study.

FIG. 9